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# Metabolomic approach determine exposure to bioactive compounds after consumption of tropical highland blackberry (*Rubus adenotrichus*) juice

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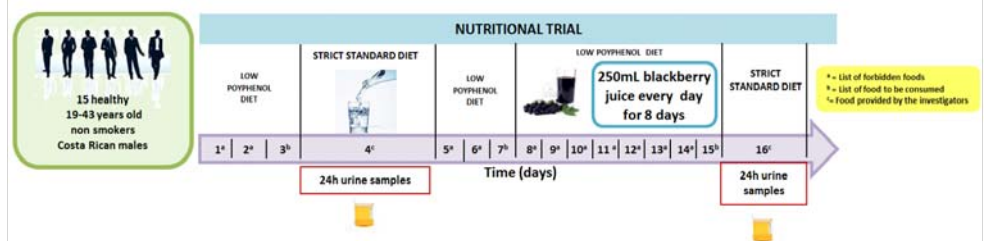
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## INTRODUCTION

Consumption of polyphenol-rich foods continues to be the focus of attention because of their putative impact on human health. Tropical highland blackberry (*Rubus adenotrichus*) juice is widely consumed from Mexico to Ecuador and represents an important source of ellagitannins and others phytochemicals for the population. Using blackberry as a model for other tropical fruits, we have shown how metabolomic profiling can be used to characterize individual exposure to bioactive molecules and their metabolites in a nutritional trial on healthy volunteers.

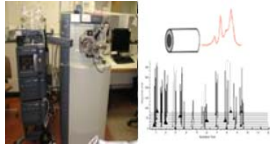
## NUTRITIONAL STUDY DESIGN

Fourteen Costa Rican men consumed for 8 days a daily dose of 250mL of a locally produced and well characterized blackberry juice, as part of a controlled diet.



## ANALYSIS

24hr urines collected before and at the end of the supplementation were analyzed with a non-targeted high-resolution mass spectrometry (UPLC-Qtof) method.



After pre-processing of LC-Qtof data, statistical analyses were applied:

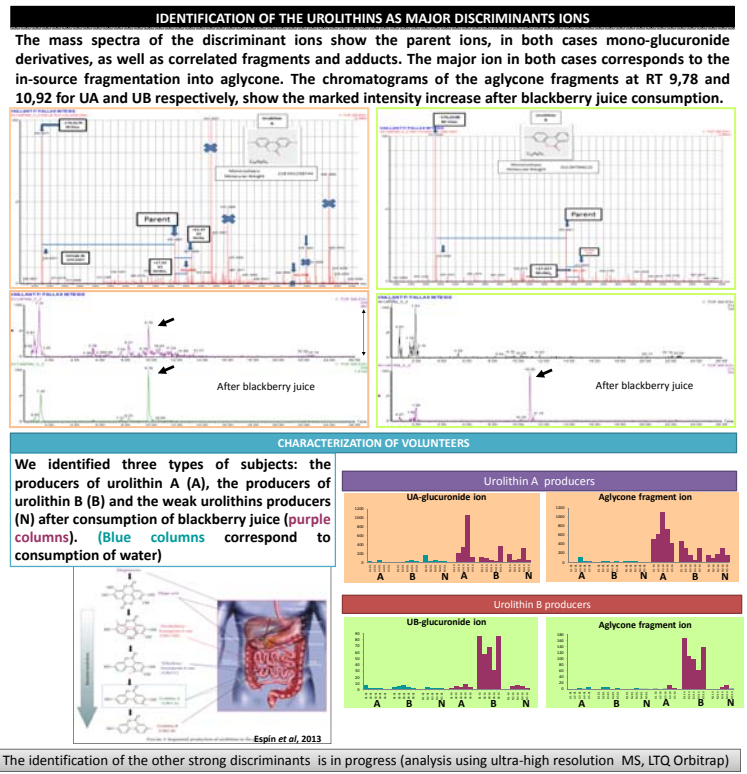
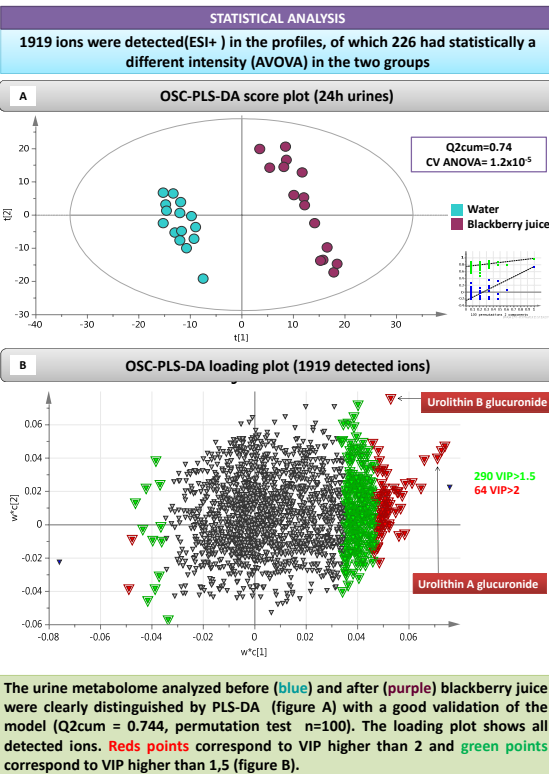
- ANOVA (R)
- PCA and OSC-PLS-DA on log-pareto data (SIMCA 13.0)

List of discriminant ions: Identification

Ion	Formula	Retention time	Abundance	Identification
115.0372	C <sub>7</sub> H <sub>7</sub> O <sub>2</sub>	9.78	High	Urolithin B
117.0372	C <sub>7</sub> H <sub>9</sub> O <sub>2</sub>	9.78	High	Urolithin B glucuronide
145.0372	C <sub>7</sub> H <sub>7</sub> O <sub>2</sub>	10.92	High	Urolithin A
147.0372	C <sub>7</sub> H <sub>9</sub> O <sub>2</sub>	10.92	High	Urolithin A glucuronide
175.0372	C <sub>7</sub> H <sub>7</sub> O <sub>2</sub>	9.78	High	Urolithin B
177.0372	C <sub>7</sub> H <sub>9</sub> O <sub>2</sub>	9.78	High	Urolithin B glucuronide
175.0372	C <sub>7</sub> H <sub>7</sub> O <sub>2</sub>	10.92	High	Urolithin A
177.0372	C <sub>7</sub> H <sub>9</sub> O <sub>2</sub>	10.92	High	Urolithin A glucuronide
191.0372	C <sub>7</sub> H <sub>7</sub> O <sub>2</sub>	9.78	High	Urolithin B
193.0372	C <sub>7</sub> H <sub>9</sub> O <sub>2</sub>	9.78	High	Urolithin B glucuronide
191.0372	C <sub>7</sub> H <sub>7</sub> O <sub>2</sub>	10.92	High	Urolithin A
193.0372	C <sub>7</sub> H <sub>9</sub> O <sub>2</sub>	10.92	High	Urolithin A glucuronide
205.0372	C <sub>7</sub> H <sub>7</sub> O <sub>2</sub>	9.78	High	Urolithin B
207.0372	C <sub>7</sub> H <sub>9</sub> O <sub>2</sub>	9.78	High	Urolithin B glucuronide
205.0372	C <sub>7</sub> H <sub>7</sub> O <sub>2</sub>	10.92	High	Urolithin A
207.0372	C <sub>7</sub> H <sub>9</sub> O <sub>2</sub>	10.92	High	Urolithin A glucuronide
221.0372	C <sub>7</sub> H <sub>7</sub> O <sub>2</sub>	9.78	High	Urolithin B
223.0372	C <sub>7</sub> H <sub>9</sub> O <sub>2</sub>	9.78	High	Urolithin B glucuronide
221.0372	C <sub>7</sub> H <sub>7</sub> O <sub>2</sub>	10.92	High	Urolithin A
223.0372	C <sub>7</sub> H <sub>9</sub> O <sub>2</sub>	10.92	High	Urolithin A glucuronide
235.0372	C <sub>7</sub> H <sub>7</sub> O <sub>2</sub>	9.78	High	Urolithin B
237.0372	C <sub>7</sub> H <sub>9</sub> O <sub>2</sub>	9.78	High	Urolithin B glucuronide
235.0372	C <sub>7</sub> H <sub>7</sub> O <sub>2</sub>	10.92	High	Urolithin A
237.0372	C <sub>7</sub> H <sub>9</sub> O <sub>2</sub>	10.92	High	Urolithin A glucuronide
251.0372	C <sub>7</sub> H <sub>7</sub> O <sub>2</sub>	9.78	High	Urolithin B
253.0372	C <sub>7</sub> H <sub>9</sub> O <sub>2</sub>	9.78	High	Urolithin B glucuronide
251.0372	C <sub>7</sub> H <sub>7</sub> O <sub>2</sub>	10.92	High	Urolithin A
253.0372	C <sub>7</sub> H <sub>9</sub> O <sub>2</sub>	10.92	High	Urolithin A glucuronide
265.0372	C <sub>7</sub> H <sub>7</sub> O <sub>2</sub>	9.78	High	Urolithin B
267.0372	C <sub>7</sub> H <sub>9</sub> O <sub>2</sub>	9.78	High	Urolithin B glucuronide
265.0372	C <sub>7</sub> H <sub>7</sub> O <sub>2</sub>	10.92	High	Urolithin A
267.0372	C <sub>7</sub> H <sub>9</sub> O <sub>2</sub>	10.92	High	Urolithin A glucuronide
281.0372	C <sub>7</sub> H <sub>7</sub> O <sub>2</sub>	9.78	High	Urolithin B
283.0372	C <sub>7</sub> H <sub>9</sub> O <sub>2</sub>	9.78	High	Urolithin B glucuronide
281.0372	C <sub>7</sub> H <sub>7</sub> O <sub>2</sub>	10.92	High	Urolithin A
283.0372	C <sub>7</sub> H <sub>9</sub> O <sub>2</sub>	10.92	High	Urolithin A glucuronide
295.0372	C <sub>7</sub> H <sub>7</sub> O <sub>2</sub>	9.78	High	Urolithin B
297.0372	C <sub>7</sub> H <sub>9</sub> O <sub>2</sub>	9.78	High	Urolithin B glucuronide
295.0372	C <sub>7</sub> H <sub>7</sub> O <sub>2</sub>	10.92	High	Urolithin A
297.0372	C <sub>7</sub> H <sub>9</sub> O <sub>2</sub>	10.92	High	Urolithin A glucuronide
311.0372	C <sub>7</sub> H <sub>7</sub> O <sub>2</sub>	9.78	High	Urolithin B
313.0372	C <sub>7</sub> H <sub>9</sub> O <sub>2</sub>	9.78	High	Urolithin B glucuronide
311.0372	C <sub>7</sub> H <sub>7</sub> O <sub>2</sub>	10.92	High	Urolithin A
313.0372	C <sub>7</sub> H <sub>9</sub> O <sub>2</sub>	10.92	High	Urolithin A glucuronide
325.0372	C <sub>7</sub> H <sub>7</sub> O <sub>2</sub>	9.78	High	Urolithin B
327.0372	C <sub>7</sub> H <sub>9</sub> O <sub>2</sub>	9.78	High	Urolithin B glucuronide
325.0372	C <sub>7</sub> H <sub>7</sub> O <sub>2</sub>	10.92	High	Urolithin A
327.0372	C <sub>7</sub> H <sub>9</sub> O <sub>2</sub>	10.92	High	Urolithin A glucuronide
341.0372	C <sub>7</sub> H <sub>7</sub> O <sub>2</sub>	9.78	High	Urolithin B
343.0372	C <sub>7</sub> H <sub>9</sub> O <sub>2</sub>	9.78	High	Urolithin B glucuronide
341.0372	C <sub>7</sub> H <sub>7</sub> O <sub>2</sub>	10.92	High	Urolithin A
343.0372	C <sub>7</sub> H <sub>9</sub> O <sub>2</sub>	10.92	High	Urolithin A glucuronide
355.0372	C <sub>7</sub> H <sub>7</sub> O <sub>2</sub>	9.78	High	Urolithin B
357.0372	C <sub>7</sub> H <sub>9</sub> O <sub>2</sub>	9.78	High	Urolithin B glucuronide
355.0372	C <sub>7</sub> H <sub>7</sub> O <sub>2</sub>	10.92	High	Urolithin A
357.0372	C <sub>7</sub> H <sub>9</sub> O <sub>2</sub>	10.92	High	Urolithin A glucuronide
371.0372	C <sub>7</sub> H <sub>7</sub> O <sub>2</sub>	9.78	High	Urolithin B
373.0372	C <sub>7</sub> H <sub>9</sub> O <sub>2</sub>	9.78	High	Urolithin B glucuronide
371.0372	C <sub>7</sub> H <sub>7</sub> O <sub>2</sub>	10.92	High	Urolithin A
373.0372	C <sub>7</sub> H <sub>9</sub> O <sub>2</sub>	10.92	High	Urolithin A glucuronide
385.0372	C <sub>7</sub> H <sub>7</sub> O <sub>2</sub>	9.78	High	Urolithin B
387.0372	C <sub>7</sub> H <sub>9</sub> O <sub>2</sub>	9.78	High	Urolithin B glucuronide
385.0372	C <sub>7</sub> H <sub>7</sub> O <sub>2</sub>	10.92	High	Urolithin A
387.0372	C <sub>7</sub> H <sub>9</sub> O <sub>2</sub>	10.92	High	Urolithin A glucuronide
401.0372	C <sub>7</sub> H <sub>7</sub> O <sub>2</sub>	9.78	High	Urolithin B
403.0372	C <sub>7</sub> H <sub>9</sub> O <sub>2</sub>	9.78	High	Urolithin B glucuronide
401.0372	C <sub>7</sub> H <sub>7</sub> O <sub>2</sub>	10.92	High	Urolithin A
403.0372	C <sub>7</sub> H <sub>9</sub> O <sub>2</sub>	10.92	High	Urolithin A glucuronide

Blackberry's metabolite database creation: Compilation of blackberry composition data

## RESULTS



## CONCLUSION

The metabolomic analysis discriminated the consumption of blackberry juice by the volunteers with more than 60 strong discriminants. Interestingly, the microbial metabolites of urolithins, urolithin A-glucuronide and urolithin B-glucuronide, were the most important discriminants but other ions currently under identification could also contribute to blackberry juice health effects. Correlations will be searched between all discriminant metabolites and the individual capacity to produce UA and UB to further investigate inter individual variation in response to blackberry juice intake.